Optimal configurations for the Heitmann-Radin energy

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(joint work with L. De Luca and M. Ponsiglione)

Sticky disc energy

Heitmann-Radin sticky disc potential

$$V_\varepsilon(r) := \begin{cases} +\infty & \text{if } r < \varepsilon\,, \\ -1 & \text{if } r = \varepsilon\,, \\ 0 & \text{if } r > \varepsilon\,. \end{cases}$$

Given a configuration of points $X := \{x_1, \dots, x_N\}$ the Heitmann-Radin energy of X is defined by

$$E_\varepsilon(X) := \frac{1}{2} \sum_{i \neq j} V_\varepsilon(|x_j - x_i|)\,.$$

Crystallization of minimizers

The minimizers X_N of E_ε among configurations with N particles lie on a triangular lattice.

R. C. Heitmann, C. Radin: The ground state for sticky disks, *J. Stat. Phys.* **22** (1980).

Problem: Study the behaviour as $N \to +\infty$, or equiv. $\varepsilon \to 0$ (rescaling $\varepsilon \sim 1/\sqrt{N}$).

Energy functional

Minimal energy per particle: The kissing number is 6.
Each bond joins two particles $\rightsquigarrow$ Energy per particle is -3.

Empirical measure: $\mu := \sum \delta_{x_i}$. We set $\mathcal{E}_\varepsilon(\mu) := E_\varepsilon(X)$.

Total energy - bulk energy $\rightsquigarrow$ Perimeter energy
Energy functional: $\mathcal{F}_\varepsilon(\mu) := \varepsilon\big(\mathcal{E}_\varepsilon(\mu) + 3\mu(\mathbb{R}^2)\big)$.

Compactness and convergence of minimizers

- If X_ε are "connected" and $\mathcal{F}_\varepsilon(\mu_\varepsilon) \leq C$, then $\varepsilon^2 \frac{\sqrt{3}}{2} \mu_\varepsilon \stackrel{*}{\rightharpoonup} \chi_\Omega$, for some set $\Omega \subset \mathbb{R}^2$ with $\chi_\Omega \in BV(\mathbb{R}^2)$.

- If X_ε are minimizers then Ω is a hexagon.

Y. Au Yeung, G. Friesecke, B. Schmidt: Minimizing atomic configurations of short range pair potentials in two dimensions: crystallization in the Wulff shape, *Calc. Var.* **44** (2012).

Remark: The hexagon has lower (asymptotic) energy than the Euclidean ball.

Local crystallization and polycrystals

Local orientation:

Let $\mathcal{F}_\varepsilon(\mu_\varepsilon) \leq C$. Most of the particles have 6 neighbors $\rightsquigarrow$ they are vertices of some ε-equilateral triangle T_ε.

Let $\theta(T_\varepsilon) \in (\frac{\pi}{3}, \frac{2}{3}\pi]$ represent the orientation of the triangle T_ε.

We set

$$\theta_\varepsilon := \sum_{T_\varepsilon} \theta(T_\varepsilon)\chi_{T_\varepsilon}.$$

Energy bound $\rightsquigarrow$ SBV bounds for θ_ε

Compactness

Theorem (De Luca, N., Ponsiglione (2018))

Let $\mathcal{F}_\varepsilon(\mu_\varepsilon) \le C$. *Then, up to a subsequence,*

$$\theta_\varepsilon(\mu_\varepsilon) \rightharpoonup \theta \qquad \text{in } SBV_{loc}(\mathbb{R}^2)\,,$$

for some $\theta = \sum_{j\in J} \theta_j \chi_{\omega_j}$ *in* $SBV(\mathbb{R}^2)$, *where* $\{\omega_j\}_j$ *is a Caccioppoli partition of* Ω .

Anisotropic perimeter

Anisotropy:

$$\varphi : \mathbb{R}^2 \to [0, +\infty) \qquad \text{(crystalline) norm on } \mathbb{R}^2$$

Wulff shape:

$$\mathcal{W}_\varphi = \{\varphi \leq 1\} \qquad \text{standard hexagon}$$

Anisotropic perimeter:

$$Per_{\varphi_\theta}(\Omega) := \int_{\partial^*\Omega} \varphi(e^{i\theta}\nu)\, d\mathcal{H}^1$$

Γ-convergence for single crystals

Theorem (De Luca, N., Ponsiglione (2018))

The following Γ-convergence result holds true:

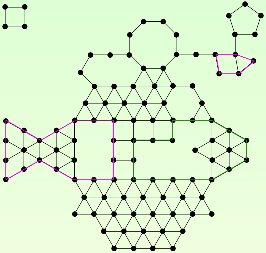
(i) *(Γ-liminf inequality) Let $\{\mu_\varepsilon\}$ satisfy the compactness result with $\theta = \bar{\theta}\chi_\Omega$ for some $\bar{\theta} \in (\frac{\pi}{3}, \frac{2}{3}\pi]$. Then*

$$\liminf_{\varepsilon \to 0} \mathcal{F}_\varepsilon(\mu_\varepsilon) \geq Per_{\varphi_{\bar{\theta}}}(\Omega).$$

(ii) *(Γ-limsup inequality) For every set $\Omega \subset \mathbb{R}^2$ of finite perimeter and for every $\bar{\theta} \in (\frac{\pi}{3}, \frac{2}{3}\pi]$, there exists a sequence $\{\mu_\varepsilon\}$ satisfying the compactness result with $\theta = \bar{\theta}\chi_\Omega$, such that*

$$\limsup_{\varepsilon \to 0} \mathcal{F}_\varepsilon(\mu_\varepsilon) \leq Per_{\varphi_{\bar{\theta}}}(\Omega).$$

Proof: Discrete Gauss-Bonnet theorem



$$
\begin{aligned}
\mathcal{F}_\varepsilon(\mu) &= \varepsilon(E_\varepsilon(X) + 3\sharp X) \\
&= Per\Big(\bigcup_{f\in F_\varepsilon(X)} f\Big) + \sum_{f\in F_\varepsilon^{\neq\Delta}(X)} \Big(Per(f) - 3\varepsilon\Big) \\
&\quad + 2\varepsilon\,\sharp\, Wires(X) + 3\varepsilon\chi(X) \\
&\geq Per\Big(\bigcup_{f\in F_\varepsilon^{\Delta}(X)} f\Big) - 3\varepsilon\,\sharp F_\varepsilon^{\neq\Delta}(X).
\end{aligned}
$$

De Luca, Friesecke: Crystallization in two dimensions and a discrete Gauss-Bonnet theorem, *J. Nonlinear Sci.* **28** (2018).

Polycrystals

Theorem (De Luca, N., Ponsiglione (2018))

The following lower and upper bounds hold true.

(i) *(Lower bound) For all $\{\mu_\varepsilon\}$ satisfying the compactness theorem, we have*

$$\liminf_{\varepsilon\to 0} \mathcal{F}_\varepsilon(\mu_\varepsilon) \geq \mathcal{H}^1(\partial^*\Omega) + \frac{1}{2}\mathcal{H}^1(\cup_j \partial^*\omega_j \setminus \partial^*\Omega)\,.$$

(ii) *(Upper bound) For every set $\Omega \subset \mathbb{R}^2$ of finite perimeter and for every $\theta \in SBV(\Omega; (\frac{\pi}{3}, \frac{2}{3}\pi])$ there exists a sequence $\{\mu_\varepsilon\}$ satisfying the compactness theorem, such that*

$$\limsup_{\varepsilon\to 0} \mathcal{F}_\varepsilon(\mu_\varepsilon) \leq \sum_j Per_{\varphi_{\theta_j}}(\omega_j)\,.$$

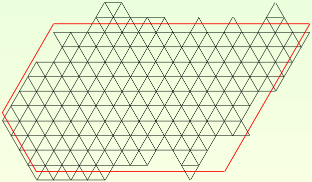
Polycrystals

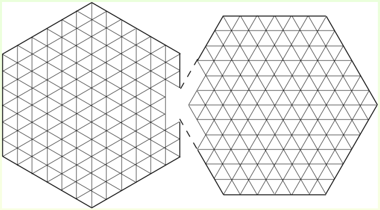
Let $\Omega \subset \mathbb{R}^2$ be given.

Minimal energy among empirical measures converging to Ω:

$$\inf_{\varepsilon^2 \frac{\sqrt{3}}{2} \mu_\varepsilon \overset{*}{\rightharpoonup} \chi_\Omega} \liminf_{\varepsilon \to 0} \varepsilon(\mathcal{E}_\varepsilon(\mu_\varepsilon) + 3\mu_\varepsilon(\mathbb{R}^2))$$

Depending on the shape of Ω, both single crystals and polycrystals could be energetically convenient:





Polycrystals

Both the lower and the upper bound are not sharp.

If two parts with different orientations touch each other along a curve, the energy might be lower than the sum of the perimeters.

Open questions

Question: Limit energy equal to $\sum_j \int_{\partial^* \omega_j} \varphi(\theta_+, \theta_-, \nu, \tau)$?
The internal variable τ represents a microscopic translation.

Blow–up technique: Global lower bounds $\rightsquigarrow$ local lower bounds
(Gauss Bonnet $\rightsquigarrow$?)

Question: Ginven a (smooth) set Ω, does local crystallization hold for large but finite N?

Open questions

Three–dimensional case:

Minimal energy per particle: The kissing number is 12.

Each bond joins two particles $\rightsquigarrow$ Energy per particle is -6.

Energy functional: $\mathcal{F}_\varepsilon(\mu) := \varepsilon^2\big(\mathcal{E}_\varepsilon(\mu) + 6\mu(\mathbb{R}^2)\big)$.

The crystallization of global minimizers is not clear.

A related problem: optimal tessellations

Problem: Find the optimal tessellation of a planar set with equilateral triangles or squares.

Setting:

$$\mathcal{A}_\varepsilon := \{\Omega \ : \ \Omega \text{ union of triangles (or squares) of sidelength } \varepsilon\}$$

Energy functional:

$$Per_\varepsilon(\Omega) := \begin{cases} Per(\Omega) & \text{if } \Omega \in \mathcal{A}_\varepsilon \\ +\infty & \text{otherwise.} \end{cases}$$

Γ-convergence

Theorem (De Luca, N., Ponsiglione (2018))

The Γ-limit of Per_ε as $\varepsilon \to 0$ is given by

$$\min_{\{\omega_j,\theta_j\}_j} \sum_j Per_{\varphi_{\theta_j}}(\omega_j)$$

where $\{\omega_j\}_j$ are Caccioppoli partitions of Ω with local orientations $\{\theta_j\}_j$.

Remark: The result does not hold if triangles/squares are replaced by hexagons.

Open questions

– Characterize the sets for which the minimum is given by a constant orientation (convex sets?).

– Tessellations in three dimensions: we can only show that

$$Per(\Omega) \leq \Gamma - \lim Per_{\varepsilon}(\Omega) \leq \min_{\{\omega_j,\theta_j\}_j} \sum_j Per_{\varphi_{\theta_j}}(\omega_j).$$

Thanks

Thanks for the attention